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I U C L I D

Data Set

Existing Chemical : ID: 25586-42-9
CAS No. : 25586-42-9
EINECS Name : tris(methylphenyl) phosphite
EC No. : 247-119-6
Molecular Formula : C₂₁H₂₁O₃P

Producer related part
Company : Rhodia UK limited
Creation date : 15.12.2005

Substance related part
Company : Rhodia UK limited
Creation date : 15.12.2005

Status :
Memo :

Printing date : 21.12.2005
Revision date :
Date of last update : 21.12.2005

Number of pages : 28

Chapter (profile) : Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile) : Reliability: without reliability, 1, 2, 3, 4
Flags (profile) : Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE),
Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1. General Information

Id 25586-42-9

Date 21.12.2005

1.0.1 APPLICANT AND COMPANY INFORMATION

Type : manufacturer
Name : Rhodia Inc.
Contact person : Glenn Simon
Date :
Street : 5171 Glenwood Avenue, Suite 402
Town : 27612 Raleigh, North Carolina
Country : United States
Phone : 919-786-9999
Telefax : 919-786-9154
Telex :
Cedex :
Email : glenn.simon@us.rhodia.com
Homepage :

21.12.2005

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

IUPAC Name : Tris(methylphenyl) phosphite
Smiles Code : Cc1ccc(cc1)OP(Oc2ccc(cc2)C)Oc3ccc(cc3)C
Molecular formula : C₂₁H₂₁O₃P
Molecular weight : 352.41
Petrol class :

15.12.2005

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type : typical for marketed substance
Substance type : organic
Physical status : liquid
Purity : > 95 % w/w
Colour : Amber
Odour : Characteristic

Remark : Marketed substance manufactured by reacting phosphorus trichloride (PCl₃) with cresol (mixture of m- and p-cresol).
Named: Tritolyl phosphite.

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Purity type : typical for marketed substance
Substance type : organic
Physical status : liquid

1. General Information

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Purity : 55 - 70 % w/w
Colour : Amber
Odour : Characteristic

Remark : Marketed substance manufactured by reacting phosphorus trichloride (PCl₃) with a mixture of cresol (mixture of m- and p-cresol) and phenol.
Named: Triaryl phosphite.

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1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

Phosphorous acid, tricresyl ester

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Phosphorous acid, tris(methylphenyl) ester

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Phosphorous acid, tritolyl ester

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Tolyl phosphite

16.12.2005

Tricresol phosphite

16.12.2005

Tricresyl phosphite

16.12.2005

Tris(methylphenyl) phosphite

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Tritolyl phosphite

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TTPI

16.12.2005

1.3 IMPURITIES

Purity : typical for marketed substance
CAS-No : 1319-77-3
EC-No : 215-293-2
EINECS-Name : cresol
Molecular formula : C₇H₈O
Value : < 1.5 % w/w

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- Remark** : Marketed substance manufactured by reacting phosphorus trichloride (PCl₃) with cresol (mixture of m- and p-cresol).
Named: Tritolyl phosphite.
- 20.12.2005
- Purity** : typical for marketed substance
CAS-No :
EC-No :
EINECS-Name : Ditolylphenyl phosphite
Molecular formula : C₂₀H₁₉O₃P
Value : = 27 - 37 % w/w
- Remark** : Marketed substance manufactured by reacting phosphorus trichloride (PCl₃) with a mixture of cresol (mixture of m- and p-cresol) and phenol.
Named: Triaryl phosphite.
- 20.12.2005
- Purity** : typical for marketed substance
CAS-No :
EC-No :
EINECS-Name : Tolyldiphenyl phosphite
Molecular formula : C₁₉H₁₇O₃P
Value : = 3 - 9 % w/w
- Remark** : Marketed substance manufactured by reacting phosphorus trichloride (PCl₃) with a mixture of cresol (mixture of m- and p-cresol) and phenol.
Named: Triaryl phosphite.
- 20.12.2005
- Purity** : typical for marketed substance
CAS-No : 101-02-0
EC-No : 202-908-4
EINECS-Name : triphenyl phosphite
Molecular formula : C₁₈H₁₅O₃P
Value : < 1 % w/w
- Remark** : Marketed substance manufactured by reacting phosphorus trichloride (PCl₃) with a mixture of cresol (mixture of m- and p-cresol) and phenol.
Named: Triaryl phosphite.
- 20.12.2005
- Purity** : typical for marketed substance
CAS-No : 1319-77-3
EC-No : 215-293-2
EINECS-Name : cresol
Molecular formula : C₇H₈O
Value : < 1 % w/w
- Remark** : Marketed substance manufactured by reacting phosphorus trichloride (PCl₃) with a mixture of cresol (mixture of m- and p-cresol) and phenol.
Named: Triaryl phosphite.
- 21.12.2005
- Purity** : typical for marketed substance
CAS-No : 108-95-2
EC-No : 203-632-7
EINECS-Name : phenol
Molecular formula : C₆H₆O
Value : < .5 % w/w
- Remark** : Marketed substance manufactured by reacting phosphorus trichloride

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(PCI3) with a mixture of cresol (mixture of m- and p-cresol) and phenol.
Named: Triaryl phosphite.

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1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1. General Information

Id 25586-42-9
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1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

Type of search : Internal and External
Chapters covered : 2
Date of search : 28.10.2005

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Type of search : Internal and External
Chapters covered : 3, 4, 5
Date of search : 28.10.2005

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1.13 REVIEWS

2. Physico-Chemical Data

Id 25586-42-9

Date 21.12.2005

2.1 MELTING POINT

Value : = 52 °C
Sublimation :
Method :
Year :
GLP :
Test substance : other TS: tri(p-cresyl)phosphite

Reliability : (2) valid with restrictions
Cited in standard data source.
Flag : Critical study for SIDS endpoint
19.12.2005 (1) (2)

Value : = 24 - 25 °C
Sublimation :
Method :
Year :
GLP :
Test substance : no data

Reliability : (4) not assignable
Cited in SDS/MSDS.
20.12.2005 (3) (4)

Value : = 167 °C
Sublimation :
Method : other: calculated
Year :
GLP :
Test substance : other TS

Method : Estimated with MPBPWIN programme v1.41, US-EPA/Syracuse Research Corporation.

Test substance : Estimated from the molecular structure.
SMILES : Cc1ccc(cc1)OP(Oc2ccc(cc2)C)Oc3ccc(cc3)C
CHEM : Phosphorous acid, tris(methylphenyl) ester
CAS NUM: 025586-42-9

Reliability : (2) valid with restrictions
Accepted calculation method.
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2.2 BOILING POINT

Value : = 240 - 243 °C at 13.3 hPa
Decomposition :
Method :
Year :
GLP :
Test substance : other TS: tri(m-cresyl)phosphite

Result : Boiling point = 235-238 °C at 9.3 hPa
Boiling point = 240-243 °C at 13.3 hPa

Reliability : (2) valid with restrictions
Cited in standard data source.

Flag : Critical study for SIDS endpoint
19.12.2005 (1) (5)

2. Physico-Chemical Data

Id 25586-42-9

Date 21.12.2005

Value : = 235 - 238 °C at 9.3
Decomposition :
Method :
Year :
GLP :
Test substance : other TS: tri(m-cresyl)phosphite

Reliability : (2) valid with restrictions
Cited in standard data source.

19.12.2005

(1) (6)

Value : = 216 °C at 7.3 hPa
Decomposition :
Method :
Year :
GLP :
Test substance : other TS: tri(m-cresyl)phosphite

Reliability : (2) valid with restrictions
Cited in standard data source.

19.12.2005

(1) (7)

Value : = 217 °C at 6.7 hPa
Decomposition :
Method :
Year :
GLP :
Test substance : other TS: tri(m-cresyl)phosphite

Reliability : (2) valid with restrictions
Cited in standard data source.

19.12.2005

(1) (8)

Value : = 188 °C at 1.3 hPa
Decomposition :
Method :
Year :
GLP :
Test substance : other TS: tri(m-cresyl)phosphite

Reliability : (2) valid with restrictions
Cited in standard data source.

19.12.2005

(1) (9)

Value : = 174 °C at .23 hPa
Decomposition :
Method :
Year :
GLP :
Test substance : other TS: tri(m-cresyl)phosphite

Reliability : (2) valid with restrictions
Cited in standard data source.

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(1) (10)

Value : = 135 °C at .13 hPa
Decomposition :
Method :
Year :
GLP :
Test substance : other TS: tri(m-cresyl)phosphite

2. Physico-Chemical Data

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Date 21.12.2005

Reliability	: (2) valid with restrictions Cited in standard data source.	
19.12.2005		(1) (11)
Value	: = 250 °C at 13.3 hPa	
Decomposition	:	
Method	:	
Year	:	
GLP	:	
Test substance	: other TS: tri(p-cresyl)phosphite	
Reliability	: (2) valid with restrictions Cited in standard data source.	
Flag	: Critical study for SIDS endpoint	
19.12.2005		(1) (11)
Value	: = 250 - 255 °C at 13.3 hPa	
Decomposition	:	
Method	:	
Year	:	
GLP	:	
Test substance	: other TS: tri(p-cresyl)phosphite	
Reliability	: (2) valid with restrictions Cited in standard data source.	
19.12.2005		(1) (5)
Value	: = 236 - 239 °C at 9.3 hPa	
Decomposition	:	
Method	:	
Year	:	
GLP	:	
Test substance	: other TS: tri(p-cresyl)phosphite	
Reliability	: (2) valid with restrictions Cited in standard data source.	
19.12.2005		(1) (6)
Value	: = 230 °C at 3.3 hPa	
Decomposition	:	
Method	:	
Year	:	
GLP	:	
Test substance	: other TS: tri(p-cresyl)phosphite	
Reliability	: (2) valid with restrictions Cited in standard data source.	
19.12.2005		(1) (7)
Value	: = 194 °C at 1.3 hPa	
Decomposition	:	
Method	:	
Year	:	
GLP	:	
Test substance	: other TS: tri(p-cresyl)phosphite	
Reliability	: (2) valid with restrictions Cited in standard data source.	
19.12.2005		(1) (9)
Value	: = 198 - 200 °C at 1.1 hPa	

2. Physico-Chemical Data

Id 25586-42-9

Date 21.12.2005

Decomposition	:		
Method	:		
Year	:		
GLP	:		
Test substance	:	other TS: tri(p-cresyl)phosphite	
Reliability	:	(2) valid with restrictions Cited in standard data source.	
19.12.2005			(1) (8)
Value	:	= 215 - 220 °C at .4 hPa	
Decomposition	:		
Method	:		
Year	:		
GLP	:		
Test substance	:	other TS: tri(p-cresyl)phosphite	
Reliability	:	(2) valid with restrictions Cited in standard data source.	
19.12.2005			(1) (12)
Value	:	= 175 °C at .4 hPa	
Decomposition	:		
Method	:		
Year	:		
GLP	:		
Test substance	:	other TS: tri(p-cresyl)phosphite	
Reliability	:	(2) valid with restrictions Cited in standard data source.	
19.12.2005			(1) (13)
Value	:	= 180 °C at .24 hPa	
Decomposition	:		
Method	:		
Year	:		
GLP	:		
Test substance	:	other TS: tri(p-cresyl)phosphite	
Reliability	:	(2) valid with restrictions Cited in standard data source.	
19.12.2005			(1) (10)
Value	:	= 360 - 361 °C at 1013 hPa	
Decomposition	:		
Method	:		
Year	:		
GLP	:		
Test substance	:	no data	
Reliability	:	(4) not assignable Cited in SDS/MSDS.	
20.12.2005			(3) (4)
Value	:	= 446 °C at 1013 hPa	
Decomposition	:		
Method	:	other: calculated	
Year	:		
GLP	:		
Test substance	:		
Method	:	Estimated with MPBPWIN programme v1.41, US-EPA/Syracuse Research	

2. Physico-Chemical Data

Id 25586-42-9

Date 21.12.2005

Test substance : Corporation.
: Estimated from the molecular structure.
SMILES : Cc1ccc(cc1)OP(Oc2ccc(cc2)C)Oc3ccc(cc3)C
CHEM : Phosphorous acid, tris(methylphenyl) ester
CAS NUM: 025586-42-9

Reliability : (2) valid with restrictions
Accepted calculation method.

Flag : Critical study for SIDS endpoint
20.12.2005

2.3 DENSITY

Type : relative density
Value : = 1.127 at 20 °C
Method :
Year :
GLP :
Test substance : other TS: tri(m-cresyl)phosphite

Remark : Density relative to water at 20°C.
Reliability : (2) valid with restrictions
Cited in standard data source.

19.12.2005

(1) (8)

Type : relative density
Value : = 1.1195 at 25 °C
Method :
Year :
GLP :
Test substance : other TS: tri(m-cresyl)phosphite

Remark : Density relative to water at 25°C.
Reliability : (2) valid with restrictions
Cited in standard data source.

19.12.2005

(1) (9)

Type : relative density
Value : = 1.126 at 25 °C
Method :
Year :
GLP :
Test substance : other TS: tri(m-cresyl)phosphite

Result : Temperature: 15°C 25°C 45°C 65°C
Relative density: 1.134 1.126 1.110 1.094
(Density relative to water at 4°C)

Reliability : (2) valid with restrictions
Cited in standard data source.

19.12.2005

(1) (10)

Type : relative density
Value : = 1.1285 at 25 °C
Method :
Year :
GLP :
Test substance : other TS: tri(m-cresyl)phosphite

Remark : Density relative to water at 25°C.
Reliability : (2) valid with restrictions
Cited in standard data source.

2. Physico-Chemical Data

Id 25586-42-9

Date 21.12.2005

19.12.2005

(1) (6)

Type : relative density
Value : = 1.128 at 20 °C
Method :
Year :
GLP :
Test substance : other TS: tri(p-cresyl)phosphite

Remark : Density relative to water at 20°C.
Reliability : (2) valid with restrictions
 Cited in standard data source.

19.12.2005

(1) (8)

Type : relative density
Value : = 1.1287 at 20 °C
Method :
Year :
GLP :
Test substance : other TS: tri(p-cresyl)phosphite

Remark : Density relative to water at 20°C.
Reliability : (2) valid with restrictions
 Cited in standard data source.

19.12.2005

(1) (14)

Type : relative density
Value : = 1.1107 at 25 °C
Method :
Year :
GLP :
Test substance : other TS: tri(p-cresyl)phosphite

Remark : Density relative to water at 25°C.
Reliability : (2) valid with restrictions
 Cited in standard data source.

19.12.2005

(1) (9)

Type : relative density
Value : = 1.127 at 25 °C
Method :
Year :
GLP :
Test substance : other TS: tri(p-cresyl)phosphite

Result : Temperature: 15°C 25°C 45°C 65°C
 Relative density: 1.134 1.127 1.111 1.095
 (Density relative to water at 4°C)

Reliability : (2) valid with restrictions
 Cited in standard data source.

19.12.2005

(1) (10)

Type : relative density
Value : = 1.1313 at 25 °C
Method :
Year :
GLP :
Test substance : other TS: tri(p-cresyl)phosphite

Remark : Density relative to water at 25°C.
Reliability : (2) valid with restrictions
 Cited in standard data source.

2. Physico-Chemical Data

Id 25586-42-9

Date 21.12.2005

19.12.2005

(1) (6)

Type : relative density
Value : = 1.18 at 20 °C
Method :
Year :
GLP :
Test substance : no data

Reliability : (4) not assignable
Cited in SDS/MSDS.

20.12.2005

(3) (4)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : = .000000475 hPa at 25 °C
Decomposition :
Method : other (calculated)
Year :
GLP :
Test substance :

Method : Estimated with MPBPWIN programme v1.41, US-EPA/Syracuse Research Corporation.
Result : Vapor Pressure Estimations (25 deg C):
(Using BP: 445.65 deg C (estimated))
(Using MP: 52.00 deg C (user entered))
VP: 2.75E-008 mm Hg (Antoine Method)
VP: 3.56E-007 mm Hg (Modified Grain Method)
VP: 7.16E-007 mm Hg (Mackay Method)
Selected VP: 3.56E-007 mm Hg (Modified Grain Method)
Test substance : Estimated from the molecular structure.
SMILES : Cc1ccc(cc1)OP(Oc2ccc(cc2)C)Oc3ccc(cc3)C
CHEM : Phosphorous acid, tris(methylphenyl) ester
CAS NUM: 025586-42-9
Reliability : (2) valid with restrictions
Accepted calculation method.
Flag : Critical study for SIDS endpoint
19.12.2005

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water
Log pow : = 8.3 at 25 °C
pH value :
Method : other (calculated)
Year :
GLP :
Test substance :

Method : Estimated with KOWPWIN programme v1.67, US-EPA/Syracuse Research Corporation.
Test substance : Estimated from the molecular structure.
SMILES : Cc1ccc(cc1)OP(Oc2ccc(cc2)C)Oc3ccc(cc3)C
CHEM : Phosphorous acid, tris(methylphenyl) ester

2. Physico-Chemical Data

Id 25586-42-9

Date 21.12.2005

Reliability : CAS NUM: 025586-42-9
: (2) valid with restrictions
Accepted calculation method.
Flag : Critical study for SIDS endpoint
19.12.2005

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : = .00089 mg/l at 25 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method : other: calculated
Year :
GLP :
Test substance :

Method : Estimated with WSKOW programme v1.41, US-EPA/Syracuse Research Corporation.

Result : Log Kow (estimated) : 8.27
Log Kow (experimental): not available from database
Log Kow used by Water solubility estimates: 8.27

Equation Used to Make Water Sol estimate:

$\text{Log S (mol/L)} = 0.693 - 0.96 \log \text{Kow} - 0.0092(\text{Tm} - 25) - 0.00314 \text{ MW} + \text{Correction}$

Melting Pt (Tm) = 52.00 deg C (Use Tm = 25 for all liquids)

Correction(s): Value

No Applicable Correction Factors

Test substance : Log Water Solubility (in moles/L) : -8.598
Water Solubility at 25 deg C (mg/L): 0.00089
: Estimated from the molecular structure.
SMILES : Cc1ccc(cc1)OP(Oc2ccc(cc2)C)Oc3ccc(cc3)C
CHEM : Phosphorous acid, tris(methylphenyl) ester
CAS NUM: 025586-42-9

Reliability : (2) valid with restrictions
Accepted calculation method.
Flag : Critical study for SIDS endpoint
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2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value : = 120 °C
Type : closed cup
Method :

2. Physico-Chemical Data

Id 25586-42-9

Date 21.12.2005

Year :
GLP : no data
Test substance : no data

Reliability : (4) not assignable
Cited in SDS/MSDS.

19.12.2005

(3) (4)

Value : = 255.4 °C
Type :
Method : other: calculated
Year :
GLP :
Test substance :

Method : Calculated using Advanced Chemistry Development (ACD/Labs) Software V8.14 ((C) 1994-2005 ACD/Labs).

Result : Flash point = 255.4 +/- 28.7 deg C

Test substance : Molecular structure of Tris(m-tolyl) phosphite.

Reliability : (2) valid with restrictions
Accepted calculation method.

19.12.2005

Value : = 253 °C
Type :
Method : other: calculated
Year :
GLP :
Test substance :

Method : Calculated using Advanced Chemistry Development (ACD/Labs) Software V8.14 ((C) 1994-2005 ACD/Labs).

Result : Flash point = 253.0 +/- 28.7 deg C

Test substance : Molecular structure of Tris(p-tolyl) phosphite.

Reliability : (2) valid with restrictions
Accepted calculation method.

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2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

Value : = 21.17 - mPa s (dynamic) at 25 °C
Result :

2. Physico-Chemical Data

Id 25586-42-9

Date 21.12.2005

Method :
Year :
GLP :
Test substance : other TS: tri(m-cresyl)phosphite

Result : Temperature: 15°C 25°C 45°C 65°C
Viscosity (mPa.s): 37.55 21.17 9.132 5.075

Reliability : (2) valid with restrictions
Cited in standard data source.

19.12.2005

(1) (10)

Value : = 20.17 - mPa s (dynamic) at 25 °C

Result :
Method :
Year :
GLP :
Test substance : other TS: tri(p-cresyl)phosphite

Result : Temperature: 15°C 25°C 45°C 65°C
Viscosity (mPa.s): 35.23 20.17 8.794 5.017

Reliability : (2) valid with restrictions
Cited in standard data source.

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(1) (10)

2.14 ADDITIONAL REMARKS

3. Environmental Fate and Pathways

Id 25586-42-9

Date 21.12.2005

3.1.1 PHOTODEGRADATION

Type : air
Light source :
Light spectrum : nm
Relative intensity : based on intensity of sunlight
INDIRECT PHOTOLYSIS
Sensitizer : OH
Conc. of sensitizer : 1500000 molecule/cm³
Rate constant : = .0000000000136991 cm³/(molecule*sec)
Degradation : = 50 % after .8 day(s)

Method : Estimated with AOPWIN programme v1.91, US-EPA/Syracuse Research Corporation.
Result : OVERALL OH Rate Constant = 13.6991 E-12 cm³/molecule-sec
HALF-LIFE = 0.781 Days (12-hr day; 1.5E6 OH/cm³)
HALF-LIFE = 1.171 Days (24-hr day; 0.5E6 OH/cm³)
Test substance : Estimated from the molecular structure.
SMILES : Cc1ccc(cc1)OP(Oc2ccc(cc2)C)Oc3ccc(cc3)C
CHEM : Phosphorous acid, tris(methylphenyl) ester
CAS NUM: 025586-42-9
Reliability : (2) valid with restrictions
Accepted calculation method.
Flag : Critical study for SIDS endpoint
19.12.2005

3.1.2 STABILITY IN WATER

Type : abiotic
t1/2 pH4 : at °C
t1/2 pH7 : at °C
t1/2 pH9 : at °C
Deg. product :
Method :
Year :
GLP :
Test substance : other TS

Result : The three phosphites can be decomposed nearly completely in water in 1 to 3 hours at 80°C to 100°C. Partial decomposition may be effected in 15 to 60 minutes at 60°C to 80°C.
Determination of inorganic phosphite-phosphorus at various stages of hydrolysis usually showed an approximately close parallelism with the respective cresols, indicating the simple decomposition of the phosphites in water into the cresols on the one hand and phosphorous acid on the other.
Test condition : Experiments were made with 1 % suspension of each of the phosphorous acid esters (tri(o-cresyl) phoshite, tri(m-cresyl) phoshite and tri(p-cresyl) phoshite) in water for a definite length of time and at a constant temperature.
At the end of the hydrolysis period, the suspension was filtered through hard filter paper and the cresols and the inorganic phosphite-phosphorus determined in the filtrate.
Phosphite-phosphorus was first converted to phosphate-phosphorus before it can be measured.
Test substance : Tri(o-cresyl) phoshite, Tri(m-cresyl) phoshite and Tri(p-cresyl) phoshite.
Reliability : (4) not assignable
Experimental details are missing. Unsuitable test system.

3. Environmental Fate and Pathways

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(15)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media : other: air - water - soil - sediment
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: calculated
Year :

Method : Estimated with EPIWIN programme v3.12, US-EPA/Syracuse Research Corporation.

Result :

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.0983	18.7	1000
Water	1.32	1.44e+003	1000
Soil	33.9	2.88e+003	1000
Sediment	64.7	1.3e+004	0

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	1.08	18.7	1000
Water	0.446	1.44e+003	0
Soil	76.6	2.88e+003	0
Sediment	21.9	1.3e+004	0

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	1.8e-006	18.7	0
Water	2	1.44e+003	1000
Soil	0.000127	2.88e+003	0
Sediment	98	1.3e+004	0

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	4.26e-008	18.7	0
Water	0.00197	1.44e+003	0
Soil	99.9	2.88e+003	1000
Sediment	0.0965	1.3e+004	0

Test condition : INPUTS:

Chem Name : Phosphorous acid, tris(methylphenyl) ester
Molecular Wt: 352.37
Henry's LC : 7.28e-007 atm-m3/mole (Henrywin program)
Vapor Press : 3.56e-007 mm Hg (Mpbpwin program)

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Liquid VP : 6.58e-007 mm Hg (super-cooled)
Melting Pt : 52 deg C (user-entered)
Log Kow : 8.27 (Kowwin program)
Soil Koc : 7.63e+007 (calc by model)

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):

Air: 18.74

Water: 1440

Soil: 2880

Sediment: 1.296e+004

(Biowin estimate: 2.196 (months))

Test substance

: Estimated from the molecular structure.

SMILES : Cc1ccc(cc1)OP(Oc2ccc(cc2)C)Oc3ccc(cc3)C

CHEM : Phosphorous acid, tris(methylphenyl) ester

CAS NUM: 025586-42-9

Reliability

: (2) valid with restrictions

Accepted calculation method.

Flag

: Critical study for SIDS endpoint

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3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4. Ecotoxicity

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4.1 ACUTE/PROLONGED TOXICITY TO FISH

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5. Toxicity

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5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type : other: ALD
Value : ca. 11000 mg/kg bw
Species : rat
Strain : other: ChR-CD
Sex : male
Number of animals : 7
Vehicle : other: corn oil
Doses : 670, 2250, 3400, 5000, 7500, 11000, 17000 mg/kg bw
Method : other: no data
Year : 1972
GLP : no
Test substance : other TS

Remark : No information is given on number of animals tested per dose. The format of the mortality data for the two highest doses implies use of only one animal per dose level.

Result : No necropsies appear to have been carried out.
Mortalities:
17000 mg/kg: Death 4h after dosing
11000 mg/kg: Death 1 day after dosing

Clinical signs:
3400 mg/kg and above: Stained perinal area 1-3 days after dosing
7500 mg/kg and above: ruffled fur for 5 days, weight loss 2-7 days after dosing.
11000 mg/kg and above: tremors

Test condition : Approximate Lethal Dose (ALD): 11000 mg/kg bw
A single dose of the test material was administered as a solution in corn oil, by intragastric intubation to young adult ChR-CD male rats. Survivors were sacrificed 14 days later.

Test substance : m,p-Tritolyl phosphite, purity not stated

Reliability : (4) not assignable
Insufficient information on method is available in the test report to assess reliability. Endpoints studied and number of animal used appear to be fewer than required in guideline studies.

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5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5. Toxicity

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Species : guinea pig
Concentration : .1 g
Exposure : no data
Exposure time : 72 hour(s)
Number of animals : 10
Vehicle : other: none
PDII :
Result : irritating
Classification : irritating
Method : other: no data
Year : 1969
GLP : no
Test substance : other TS

Result : A mild reaction only was seen in all test animals at 24 hours.

At 72 hours, strong irritation (erythema and oedema) had developed in all test animals, spreading well beyond the site of application (3-5 x 4-6 cm).

No calculation of PDII was made, but the test material was judged to be irritant.

Test condition : 0.05 ml of undiluted test substance was applied to the shaved intact shoulder skin (ca, 2x2 cm) of 10 male albino guinea pigs. No information is available to indicate whether the test material was washed off after 24 hours.

Test substance : Tritolyl Phosphite, lot and purity not stated. Impurities: traces of cresols and phosphorous trichloride

Reliability : (4) not assignable
The study used a lower quantity of test material than would be used in a guideline study, for shorter duration and in guinea pigs, not rabbits. The results are therefore difficult to assess.

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5.2.2 EYE IRRITATION

5.3 SENSITIZATION

Type : no data
Species : guinea pig
Concentration : 1st: Induction 1 % intracutaneous
2nd: Challenge 25 % other
3rd: Challenge 25 % other
Number of animals : 20
Vehicle : other: dimethyl phthalate
Result : not sensitizing
Classification : not sensitizing
Method : other
Year : 1969
GLP : no
Test substance : other TS

Result : Topical applications with 50% test substance in Dimethyl phthalate were discontinued after 2 days due to severe reactions extending well beyond the application site.

Skin reactions at the first challenge showed strong erythema and oedema in all 5 test animals with intact skin, and 4/5 animals with abraded skin. Reactions were somewhat reduced at the second challenge.

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Test condition

The study concluded that the challenge reactions appeared to be due to primary irritancy rather than to an allergic reaction.
: Two topical applications were made to the abraded skin of five animals using 50% concentration of test substance in dimethyl phthalate.

Five animals received four 0.1 ml intradermal injections of 1% test substance in DMP over a three-week period.

A first challenge test was made two weeks after the final intradermal injection. Test and control animals received topical applications of 25% test material in DMP to intact and abraded skin. The intact skin of previously untreated control animals was treated with 1, 5, 10 and 25% test substance in DMP.

Test substance

Four weeks later, a second challenge test was performed.
: Tritolyl phosphite, lot number and purity not stated. Impurities: traces of cresols and phosphorous trichloride.

Reliability

: (4) not assignable
There is insufficient detail in the study report to assess the validity of the conclusion that positive reactions seen at challenge were due to primary irritancy rather than to sensitisation.

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5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

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10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT